

# Motion and Ionization Equilibrium of Hydrogen Atoms in Superstrong Magnetic Field

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## Abstract

We study the effects of finite proton mass on the energy levels of hydrogen atoms moving transverse to a superstrong magnetic field  $B$  with generalized pseudomomentum  $K_{\perp}$ . Field strengths of order  $B \sim 10^{12}$  Gauss are typically found on the surfaces of neutron stars, but we also study the regime  $B \gtrsim B_{crit} = 4.23 \times 10^{13}$  Gauss, where the Landau excitation energy of the proton is large. We adopt two different approaches to the two-body problem in strong magnetic field, and obtain an approximate, but complete solution of the atomic energy as a function of  $B$  and  $K_{\perp}$ . We show that, for  $B \gg B_{crit}$ , there is an orthogonal set of bound states, which do not have any Landau excitation contribution in their energies. The states with very large  $K_{\perp}$  have small binding energy and small transverse velocity, but are nevertheless distinct

from the fully ionized states. The final results for the excitation energies are given in the form of analytical fitting formulae.

The generalized Saha equation for the ionization-recombination equilibrium of hydrogen gas in the presence of a superstrong magnetic field is then derived. Although the maximum transverse velocity of a bound atom decreases as  $B$  increases, the statistical weight due to transverse motion is actually increased by the strong magnetic field. For astrophysically interesting case of relatively low density and temperature, we obtain analytic approximations for the partition functions. The highly excited bound states have a smaller statistical weight than the fully ionized component.

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## I. INTRODUCTION

It is well known that a superstrong magnetic field of order  $B \gtrsim 10^{12}$  Gauss, typically found on the surfaces of neutron stars, can dramatically change the structure of neutral atoms and other bound states (see, e.g., Ref. [1] for an early review and Ref. [2] for a recent text on atoms in strong magnetic fields). The atomic unit  $B_o$  for the magnetic field strength and a dimensionless parameter  $b$  are

$$B_o = \frac{m_e^2 c^3}{\hbar^3} = 2.35 \times 10^9 \text{ G}; \quad b \equiv \frac{B}{B_o}. \quad (1.1)$$

When  $b \gg 1$ , the cyclotron energy of the electron  $\hbar\omega_e = \hbar(eB/m_e c) = 11.58 B_{12} \text{ keV}$ , where  $B_{12}$  is the magnetic field strength in units of  $10^{12} \text{ G}$ , is much larger than the typical Coulomb energy, thus the Coulomb forces act as a perturbation to the magnetic forces on the electrons, and at most temperatures the electrons settle into the ground Landau level. Because of the extreme confinement of electrons in the transverse direction, the Coulomb force becomes much more effective for binding electrons in the parallel direction. The atom has a cigar-like structure. Moreover, it is possible for these elongated atoms to form molecular chains by covalent bonding along the field direction.

Hydrogen atoms in strong magnetic field have been studied extensively [3–7]. We have also recently completed a study of the electronic structure of hydrogen molecules and chains in the strong field regime ( $b \gg 1$ ) [8]. However, in many of these studies, the center-of-mass (CM) effects of the proton motion have been neglected. In the case of the hydrogen atom, although significant effort has been devoted to calculating the energy levels of an electron in the static Coulomb potential of a *fixed* proton (infinite mass) to a high precision and for arbitrary magnetic field strength [6,7], the two-body problem in strong magnetic field, including the effects of finite proton mass, has been studied in detail only recently (e.g., [9,10]). In this paper we focus on the hydrogen atom, but discuss those aspects which are important for application to molecules in very strong fields (we shall study molecular excitation levels in a later paper [11]).

A free electron confined to the ground Landau level, the usual case for  $b \gg 1$ , does not move perpendicular to the magnetic field. Such motion is necessarily accompanied by Landau excitations. When the electron (still in the Landau ground state) combines with a proton, the mobility of the neutral atom across the field depends on the ratio of the atomic excitation energy and the Landau excitation energy  $\hbar\omega_p = \hbar eB/(m_p c)$  for the proton. As the typical Coulomb excitation is  $(\ln b)$  in atomic units, it is convenient to define a critical field strength  $B_{crit}$  via

$$b_{crit} \equiv \frac{m_p}{m_e} \ln b_{crit} = 1.80 \times 10^4; \quad B_{crit} = b_{crit} B_o = 4.23 \times 10^{13} \text{ G}. \quad (1.2)$$

For  $B \ll B_o$  (terrestrial conditions) the Landau energies of both electron and proton are minor perturbations and one can construct wave packets that mimic the classical motion of a neutral atom across the field. In this case the internal structure of the atom or molecule is coupled to the center-of-mass motion only through a “motional Stark effect” (see Sec. II). In the opposite limit of  $B \gg B_{crit} \gg B_o$ , the Landau energies are larger than the Coulomb excitation energy, and both electron and proton (in the atom) are in the Landau ground state at reasonable temperatures. In this case, quantum mechanics cannot mimic classical motion. The canonical field strengths of radio pulsars, with  $B$  slightly less than  $B_{crit}$ , present an intermediate case. However, at all field strengths one can introduce a pseudomomentum  $\mathbf{K}_\perp$  perpendicular to the field and, in principle, find the bound-state energy  $\mathcal{E}$  as a function of  $\mathbf{K}_\perp$ . One question of interest is the range of  $K_\perp$  for which  $\mathcal{E}$  increases linearly with  $K_\perp^2$  (as it does for ordinary kinetic energy); but in any case  $\mathcal{E}(K_\perp)$  is needed to evaluate the Saha equation for the equilibrium between neutral and ionized hydrogen (Sec. V). Previous treatments [12–15] of the ionization equilibrium in strong magnetic fields did not properly take account of the non-trivial effects of atomic motion. States with large  $K_\perp$ , where velocity decreases with increasing  $K_\perp$  (see Ref. [10] and our Eq. [3.29]) are of particular interest, especially for  $B$  larger than  $B_{crit}$ .

The separation of the center-of-mass (CM) motion of a bound state in the presence of a magnetic field has been studied previously based on the conserved pseudomomentum (e.g.,

[16–21]). We briefly review and clarify this pseudomomentum scheme in Sec. II. When  $B \ll B_{crit}$ , perturbation calculations for hydrogen atom motion (e.g., [19,22,23]) are valid over a wide range of  $K_{\perp}$  values and lead to interesting phenomena such as bent trajectories [23]. Model atmospheres can be affected by details of the transverse motion (e.g., [24,25]). Some accurate numerical calculations for general  $K_{\perp}$  and for several values of  $B$  (but all below  $B_{crit}$ ) are now available [9,10], but we concentrate on the  $B \gtrsim B_{crit}$  regime in Sec. III–IV. A different approach to the two-body problem (for positronium atom) in the superstrong field regime  $b \gg 1$  has been developed in [26].

Our purpose in this paper is not to obtain accurate energy spectra of a moving hydrogen atom in certain limited regimes, as have been done in most of the papers mentioned above; rather, we seek complete (though approximate) solutions of the two-body problem for a wide range of parameter space, including  $B$  just below  $B_{crit}$  (a common case for neutron stars), but especially for  $B > B_{crit}$  (in case  $B \gtrsim 10^{14}$  G exists in some neutron stars, as has been suggested recently [27–29]). Our emphasis is on finding physically meaningful approximate fitting formulae for the atomic energy of the moving atom over all relevant values of  $K_{\perp}$  (Sec. III), in order to determine the equilibrium between neutral and ionized hydrogen (Sec. V). However, in practice we shall be interested mainly in the regimes where the thermal energy  $k_B T$  is much less than the ground-state binding energy of the atom, while the gas density is much smaller than the internal density of the atom, so that the neutral and ionized fractions are of the same order of magnitude. In such cases, we are most interested in two kinds of excited bound states: (i) Those with excitation energies up to a few atomic units (comparable to  $k_B T$  but a small fraction of the binding energy) and (ii) states that are only barely bound (e.g., those with extremely large  $K_{\perp}$ ), for which one has to check whether phase-space factors make them unimportant relative to ionized hydrogen. For applications to molecules [8,11] and multi-electron atoms [30] with  $B \gg B_{crit}$ , a controversy arises regarding the “coupling” of the electron’s orbital quantum number with the Landau level of the proton (or nuclei). This is discussed in Sec. IV.

Our calculations in this paper are based on non-relativistic quantum mechanics. For

$B \gtrsim B_{rel} = (\hbar c/e^2)^2 B_o = 4.414 \times 10^{13}$  G (note that  $B_{rel}$  is close to  $B_{crit}$  only by coincidence), i.e.,  $\hbar\omega_e \gtrsim m_e c^2$ , the transverse motion of the electron becomes relativistic. However, the relativistic correction to the atomic binding energy is small as long as the electron remains non-relativistic along field direction [31]. Except as otherwise noted, we shall use atomic units (a.u.) throughout the paper, in which mass and length are expressed in units of the electron mass  $m_e$  and the Bohr radius  $a_o = \hbar^2/(m_e e^2) = 0.529 \times 10^{-8}$  cm, energy in units of 2 Rydberg  $= e^2/a_o = 2 \times 13.6$  eV; field strength is in units of  $B_o$  (Eq. [1.1]) and temperature in units of  $3.15 \times 10^5$  K.

## II. SEPARATION OF CENTER-OF-MASS MOTION: THE PSEUDOMOMENTUM APPROACH

To set the scene, we briefly review the pseudomomentum approach to the two-body problem of a hydrogen atom in a strong magnetic field [17–19]. However, the physical meaning of the pseudomomentum of the atom needs some clarification.

### A. Pseudomomentum

For a free particle of charge  $e_i$  and mass  $m_i$  in a constant magnetic field (assumed to be aligned in the  $z$ -axis), there are three momentum-like vectors: the *canonical momentum*  $\mathbf{P} = -i\hbar\nabla$ ; the *mechanical momentum*  $\mathbf{\Pi} = \mathbf{P} - e_i\mathbf{A} = m_i\mathbf{v}$ , where  $\mathbf{A}$  is the vector potential and  $\mathbf{v}$  is the velocity; and the *pseudomomentum* (or the generalized momentum), as defined by

$$\mathbf{K} = \mathbf{\Pi} + e_i\mathbf{B} \times \mathbf{r}. \quad (2.1)$$

That  $\mathbf{K}$  is a constant of motion can be easily seen from the classical equation of motion for the particle  $d\mathbf{\Pi}/dt = e_i(d\mathbf{r}/dt) \times \mathbf{B}$ . The parallel component  $K_z$  is simply the linear momentum, while the constancy of the perpendicular component  $\mathbf{K}_\perp$  is the result of the fact that the guiding center of the circular orbit of the particle does not change with time. The position vector  $\mathbf{R}_c$  of this guiding center is related to  $\mathbf{K}_\perp$  by

$$\mathbf{R}_c = \frac{\mathbf{K}_\perp \times \mathbf{B}}{e_i B^2}. \quad (2.2)$$

Mathematically, the conservation of  $\mathbf{K}$  is the result of the invariance of the Hamiltonian under a spatial translation plus a gauge transformation [18].

The existence of the integration constant  $\mathbf{K}_\perp$  or  $\mathbf{R}_c$  implies infinite degeneracy of a given Landau energy level. We can use  $\mathbf{K}$  to classify the eigenstates. However, since two components of  $\mathbf{K}_\perp$  do not commute,  $[K_x, K_y] = -ie_i B$ , only one function of  $K_x, K_y$  can be diagonalized for stationary states. This means that the guiding center of the particle can not be specified accurately. If we use  $K_x$  to classify the states, then the wavefunction has the well-known form  $e^{K_x x} \phi(y)$  [32], where the function  $\phi(y)$  is centered at  $y_c = -K_x/(e_i B)$ , as can be inferred from Eq. (2.2). The Landau degeneracy in an area  $\mathcal{A}_g = L_g^2$  is thus given by  $(L_g/2\pi) \int dK_x = (L_g/2\pi) |K_{x,g}| = \mathcal{A}_g (|e_i| B/2\pi)$ , where we have used  $K_{x,g} = -e_i B L_g$ . On the other hand, if we choose to diagonalize  $K_\perp^2 = K_x^2 + K_y^2$ , we obtain the Landau wavefunction  $W_{nm}(\mathbf{r}_\perp)$  in cylindrical coordinates [32], where  $m$  is the “orbital” quantum number (denoted by  $s$  in some references). For the ground Landau level this is

$$W_{0m}(\mathbf{r}_\perp) \equiv W_m(\rho, \theta) = \frac{1}{(2\pi m!)^{1/2} \hat{\rho}} \left( \frac{\rho}{\sqrt{2} \hat{\rho}} \right)^m \exp \left( \frac{\rho^2}{4 \hat{\rho}^2} \right) \exp(-im\theta). \quad (2.3)$$

The distance of the guiding center of the particle from the origin is given by

$$\rho_m = (2m+1)^{1/2} \hat{\rho}, \quad m = 0, 1, 2, \dots, \quad (2.4)$$

where  $\hat{\rho}$  is the cyclotron radius

$$\hat{\rho} = \left( \frac{\hbar c}{eB} \right)^{1/2} = a_o \left( \frac{B_o}{B} \right)^{1/2} = b^{-1/2} \text{ (a.u.)} = 2.57 \times 10^{-10} B_{12}^{-1/2} \text{ (cm)}. \quad (2.5)$$

The corresponding value of  $K_\perp$  is given by  $K_\perp^2 = |e_i| B (2m+1)$ . Note that  $K_\perp^2$  assumes discrete values since  $m$  is required to be an integer in order for the wavefunction to be single-valued. The degeneracy  $m_g$  of the Landau level in an area  $\mathcal{A}_g = \pi R_g^2$  is then determined by  $\rho_{m_g} \simeq (2m_g)^{1/2} \hat{\rho} = R_g$ , which again yields  $m_g = \mathcal{A}_g |e_i| B / (2\pi)$ .

We also note that  $K_\perp^2$  is related to the  $z$ -angular momentum  $J_z$ , as is evident from the  $e^{-im\theta}$  factor in the cylindrical wavefunction (Eq. [2.3]). In general, we can show that

$$J_z = xp_y - yp_x = \frac{1}{2e_i B}(\mathbf{K}_\perp^2 - \mathbf{\Pi}_\perp^2) = (m - n)\frac{|e_i|}{e_i}, \quad (2.6)$$

where we have used  $\mathbf{\Pi}_\perp^2 = |e_i|B(2n + 1)$ , and  $n$  is the quantum number for the Landau excitations.

## B. Hydrogen Atom as a Two-Body Problem

We now consider the electron-proton system. It is easy to show that even with the Coulomb interaction between the particles, the total pseudomomentum is a constant of motion

$$\mathbf{K} = \mathbf{K}_1 + \mathbf{K}_2, \quad (2.7)$$

where the subscripts 1, 2 refer to electron (charge  $-1$ ) and proton. Moreover, unlike the single particle case, here all components of  $\mathbf{K}$  commute. Thus it is natural to separate the CM motion from the internal degree of freedom, using the vector pseudomomentum  $\mathbf{K}$  as an explicit constant of motion (although we shall discuss an alternative set of basic states in Sec. IV). From Eq. (2.2) we have

$$\mathbf{R}_K = \mathbf{R}_{c1} - \mathbf{R}_{c2} = -\frac{\mathbf{K} \times \mathbf{B}}{B^2}. \quad (2.8)$$

Thus we see that  $\mathbf{K}_\perp$  is directly related to the separation  $\mathbf{R}_K$  between the guiding center of the Landau orbit of the electron and that of the proton.

Consider the energy eigenstate with a fixed  $\mathbf{K}$ . Introduce the center-of-mass coordinate  $\mathbf{R} = (m_e \mathbf{r}_1 + m_p \mathbf{r}_2)/(m_e + m_p)$  and the relative coordinate  $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ . Writing the two-body wavefunction as

$$\Psi(\mathbf{R}, \mathbf{r}) = \exp \left[ i(\mathbf{K} + \frac{1}{2}\mathbf{B} \times \mathbf{r}) \cdot \mathbf{R} \right] \phi(\mathbf{r}), \quad (2.9)$$

so that  $\Psi(\mathbf{R}, \mathbf{r})$  has a well-defined value of  $\mathbf{K}$ , while  $\exp[i(\mathbf{B} \times \mathbf{r}) \cdot \mathbf{R}/2]$  is a gauge factor, the Schrödinger equation reduces to <sup>1</sup>

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<sup>1</sup>The spin terms of the electron and the proton are not explicitly included. However, it should be



$$H\phi(\mathbf{r}) = (H_o + H')\phi(\mathbf{r}) = \mathcal{E} \phi(\mathbf{r}), \quad (2.10)$$

with

$$H_o = \frac{K_z^2}{2M} + \frac{1}{2\mu} \left( \mathbf{p} + \frac{1}{2} \mathbf{B} \times \mathbf{r} \right)^2 - \frac{1}{m_p} \mathbf{B} \cdot (\mathbf{r} \times \mathbf{p}) - \frac{1}{r}, \quad (2.11)$$

$$H' = \frac{K_\perp^2}{2M} + \frac{1}{M} (\mathbf{K} \times \mathbf{B}) \cdot \mathbf{r}, \quad (2.12)$$

where  $\mathbf{p} = -i\partial/\partial\mathbf{r}$ ,  $M = m_e + m_p \simeq m_p/m_e$  (a.u.),  $\mu = m_e m_p / M \simeq m_e$ . We will make no distinction between  $M$  and  $m_p$ , nor  $\mu$  and  $m_e$  in our following calculations. Eqs. (2.10)-(2.12) have already been derived in Refs. [16–19]. Clearly, the CM motion is coupled to the internal motion through the second term in  $H'$ , which has the form of the potential in a motion-induced electric field  $(\mathbf{K}/M) \times \mathbf{B}$ . This term represents the so called “motional Stark effect” (although such a description is not exactly accurate, since  $\mathbf{K}_\perp/M$  does not correspond to the CM velocity [20]). For small  $K_\perp$ , this effect can be considered by treating  $H'$  as a perturbation (Sec. III), but the eigenstates of  $H_o$  can in principle be used as a set of basic states for developing eigenstates of the full Hamiltonian for any value of  $K_\perp$ . However, the following transformed version of the Hamiltonian is more convenient for large  $K_\perp$ .

Motivated by the fact that  $\mathbf{K}_\perp$  measures the separation of the guiding centers of the electron and the proton, we can remove the “Stark term” by introducing a displaced coordinate  $\mathbf{r}' = \mathbf{r} - \mathbf{R}_K$ , where  $\mathbf{R}_K$  is given by Eq. (2.8). After a gauge transformation, with

$$\phi(\mathbf{r}) \rightarrow \exp \left( i \frac{m_p - m_e}{2M} \mathbf{K}_\perp \cdot \mathbf{r} \right) \phi(\mathbf{r}'), \quad (2.13)$$

the Hamiltonian becomes

$$H = \frac{K_z^2}{2M} + \frac{1}{2\mu} \left( \mathbf{p}' + \frac{1}{2} \mathbf{B} \times \mathbf{r}' \right)^2 - \frac{1}{m_p} \mathbf{B} \cdot (\mathbf{r}' \times \mathbf{p}') - \frac{1}{|\mathbf{r}' + \mathbf{R}_K|}, \quad (2.14)$$

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understood that for the ground Landau state, the zero-point Landau energy is exactly cancelled by the spin energy. Also, the abnormal intrinsic magnetic moment of the proton is neglected, since it does not play a role in our analysis.

where  $\mathbf{p}' = -i\partial/\partial\mathbf{r}'$ . This expression has been obtained in Refs. [18,19]. We shall see in Sec. III that this alternative form of the Hamiltonian is useful in the regime where  $b$  is much larger than  $b_{crit}$ , defined in Eq. (1.2).

### III. APPROXIMATE SOLUTIONS AND FITTING FORMULAE

#### A. Zeroth Order Solutions

We consider first the Hamiltonian formulation in terms of Eqs. (2.11)-(2.12). For the zeroth order Hamiltonian  $H_o$  the quantum numbers for the basic states are  $K_z$ , the number of nodes in the  $z$ -wavefunction  $\nu$ , the electron Landau level integer  $n$  and the “orbital” quantum number  $m = 0, 1, 2, \dots$ . In this paper we only consider  $b \gg 1$  and thus restrict ourselves to  $n = 0$ . The energy eigenvalues of  $H_o$  for the  $\nu = 0$  states can be written as

$$\mathcal{E}_m^{(0)}(K_z) = \frac{K_z^2}{2M} + E_m + m\frac{b}{M}, \quad (3.1)$$

where  $E_m$  is the energy of a bound electron in the fixed Coulomb potential of an infinitely massive positive charge. The last term in Eq. (3.1) for  $m \geq 1$  represents Landau energy excitations for the proton, but  $m$  is merely the “orbital” quantum number for the electron wavefunction and measures the relative  $z$ -angular momentum  $J_z = -m$ . Thus, there is no separate quantum number for the proton in this formulation. The “coupling” between the electron quantum number  $m$  and the proton Landau excitation  $mb/M$  in Eq. (3.1) results from the conservation of total pseudomomentum. The term  $E_m$  has the form (e.g., [1,8])

$$E_m \simeq -0.16A l_m^2, \quad l_m \equiv \ln \frac{b}{2m+1}, \quad (3.2)$$

where  $A$  is a coefficient which varies slowly with  $b$  and  $m$  (E.g.,  $A \simeq 1.01 - 1.3$  for  $m = 0 - 5$  when  $B_{12} = 1$ , and  $A \simeq 1.02 - 1.04$  for  $m = 0 - 5$  when  $B_{12} = 10$ ). In most formulae below, we replace  $A$  by unity; the numerical values can be found in [8,11]. The atom has a cigar-like shape, with size  $\sim \rho_m$  (cf. Eq. [2.4]) perpendicular to the field and  $L_z \sim l_m^{-1}$  along the field

direction. Note that the correction due to the reduced mass  $\mu$  could be easily incorporated by a simple scaling:

$$E_m \simeq -0.16A \frac{\mu}{m_e} \left[ \ln \left( \frac{b}{2m+1} \frac{m_e^2}{\mu^2} \right) \right]^2. \quad (3.3)$$

However, this is a small correction (of order  $m_e/m_p$ ), and will be neglected hereafter.

Equations (3.2)-(3.3) refer to the “tight-bound” states for which the number of nodes  $\nu$  of the  $z$ -wavefunction  $f(z)$  of the electron is zero. For  $\nu > 0$ , the energy eigenvalues are approximately given by [33]:

$$E_{m\nu} = -\frac{1}{2\nu_1^2} \left( 1 - \frac{4\rho_m}{\nu_1 a_o} \right), \quad \nu_1 = 1, 2, 3, \dots \quad (3.4)$$

for the odd states ( $\nu = 2\nu_1 - 1$ ), and

$$E_{m\nu} = -\frac{1}{2\nu_1^2} \left[ 1 - \frac{2}{\nu_1 \ln(a_o/\rho_m)} \right], \quad \nu_1 = 1, 2, 3, \dots \quad (3.5)$$

for the even states ( $\nu = 2\nu_1$ ). The sizes of the wavefunctions are  $\rho_m$  perpendicular to the field and  $L_z \sim \nu^2$  (a.u.) along the field. These states have much lower binding energies compared to the “tight-bound” states.

We now consider the energies and eigenstates of the atom for finite  $K_\perp$ . The two different Hamiltonian forms are discussed in Sec. III.B-C, and the general approximate expressions for the energies are then given in Sec. III.D. We focus on the “tight-bound” states only, since finite  $K_\perp$  will make the weakly-bound  $\nu > 0$  states even less bound (although in Sec. V we will include an estimate of the statistical weight of these states in the partition function of bound atom).

## B. The Perturbation Hamiltonian Formalism

For sufficiently small  $K_\perp$ , we can use standard perturbation theory to calculate the correction of energy  $\mathcal{E}$  due to  $H'$  given by Eq. (2.12) (see also [19,22,23]). Let  $\mathbf{K}_\perp$  be along the  $y$ -axis, then the  $r$ -dependent part of  $H'$  is  $K_\perp bx/M$ . We consider only  $n = 0$  and

$\nu = 0$ , so the exact eigenstates of  $H_o + H'$  are superpositions of the  $H_o$ -eigenstates with  $m = 0, 1, 2, \dots$ . The only non-zero matrix elements of  $x$  are of the form

$$\langle W_m | x | W_{m+1} \rangle = \left( \frac{m+1}{2} \right)^{1/2} \hat{\rho}, \quad (3.6)$$

and the energy differences of adjacent  $H_o$ -eigenstates are approximately given by

$$\Delta \mathcal{E}_m^{(0)} = \mathcal{E}_{m+1}^{(0)} - \mathcal{E}_m^{(0)} \simeq 0.32 l \ln \left( \frac{2m+3}{2m+1} \right) + \frac{b}{M}, \quad (3.7)$$

where  $l = l_0 \equiv \ln b$  and the factor 0.32 is an approximation to a slowly varying function of  $m$  and  $b$ . We first consider the ground state  $m = 0$ . Using  $H' = K_{\perp} b x / M + K_{\perp}^2 / (2M)$  and Eq. (3.6) we note that perturbation theory is justified if  $K_{\perp}$  is much smaller than a “perturbation limit”  $K_{\perp p}$  defined as

$$K_{\perp p} = \frac{M \Delta \mathcal{E}_0^{(0)}}{b^{1/2}} = b^{1/2} \left( 1 + \frac{M l}{\xi b} \right) \simeq b^{1/2} \left( 1 + \frac{b_{crit}}{\xi b} \right), \quad (3.8)$$

where  $\xi \sim 2.8$  is a slowly varying function of  $b$  (e.g.,  $\xi \simeq 2 - 3$  for  $B_{12} = 0.1 - 10^3$ ). For  $K_{\perp} \ll K_{\perp p}$ , the energy  $\mathcal{E}_0^{(2)}$  to be added to  $\mathcal{E}_0^{(0)}$  in Eq. (3.1) is given by second order perturbation theory (plus a diagonal term) as

$$\mathcal{E}_0^{(2)} = \frac{K_{\perp}^2}{2M} \left( 1 - \frac{b}{M \Delta \mathcal{E}_0^{(0)}} \right) = \frac{K_{\perp}^2}{2M_{\perp}}, \quad (3.9)$$

where  $M_{\perp}$  is the effective mass for the “transverse motion” of the atom,

$$M_{\perp} = M \left( 1 + \frac{\xi b}{l M} \right) \simeq M \left( 1 + \frac{\xi b}{b_{crit}} \right). \quad (3.10)$$

Thus the effective mass  $M_{\perp}$  increases with increasing  $b$ .

Similar calculations for the  $m > 0$  states yield  $\mathcal{E}_m^{(2)} = K_{\perp}^2 / (2M_{\perp m})$ , with

$$1 - \frac{M}{M_{\perp m}} \simeq \frac{b}{M} \left[ \frac{m+1}{b/M + 0.16 l_m^2 - 0.16 l_{m+1}^2} - \frac{m}{b/M + 0.16 l_{m-1}^2 - 0.16 l_m^2} \right]. \quad (3.11)$$

A convenient (but approximate) expression for the effective mass  $M_{\perp m}$  is given by

$$M_{\perp m} \simeq M + \xi_m (2m+1) \frac{b}{l_m}, \quad (3.12)$$

where  $\xi_m$  is of the same order of magnitude as  $\xi$ , but different (by a factor of a few) for different  $m$ -states. The important feature in Eqs. (3.11)-(3.12) is that the effective mass is larger for the higher- $m$  state.

The quadratic form of the effective “transverse kinetic energy” in Eq. (3.9) is valid only when it is much less than the “perturbation limit”, reached when  $K_\perp = K_{\perp p}$ . Using Eq. (3.8) and the approximation in Eq. (3.10), this kinetic energy limit becomes

$$\frac{K_{\perp p}^2}{2M_\perp} = \frac{l}{2\xi} \left( 1 + \frac{Ml}{\xi b} \right) \simeq 1.7 \left( 1 + \frac{b_{crit}}{\xi b} \right) \text{ (a.u.)}. \quad (3.13)$$

For  $b \ll b_{crit}$  (even if  $b \gg 1$ ) this limit is large compared with 1 a.u., so that the quadratic perturbation energy (or transverse kinetic energy) in Eq. (3.9) is valid for the most important (low energy) states. Moreover, from Eq. (3.10) the effective mass is close to the actually proton mass  $M$ . For superstrong fields,  $b \gg b_{crit}$ , on the other hand, the effective mass (for  $K_\perp \ll K_{\perp p}$ ) is much larger than  $M$  and the perturbation formalism already breaks down when the transverse kinetic energy is only of order 1 a.u.

At least for  $B \gg B_{crit}$ , we have to consider values of  $K_\perp$  large enough so that the perturbation treatment for the formalism in Eqs. (2.10)-(2.12) is unsuitable. For any magnetic field strength there are still eigenstates for arbitrarily large values of  $K_\perp$ , but the transformed Hamiltonian in Eqs. (2.13)-(2.14) is now more suitable for calculating the energy.

### C. The “Displaced Center” Formalism

As mentioned, Eq. (2.14) gives an alternative formulation for the Hamiltonian where  $K_\perp^2/(2M)$  does not appear explicitly, but the displacement of the electron-proton guiding centers does with  $R_K = K_\perp/b$  (in atomic units) [19,10]. We again focus only on the Landau ground state for the electron ( $n = 0$ ), but in principle we must include all  $m$ -values (with proton Landau excitation energy  $mb/M$ ) and mixing between these states. We consider first the approximation where we omit mixing, i.e., we use the diagonal matrix element of  $|\mathbf{r}' + \mathbf{R}_K|^{-1}$  for a fixed  $m$ -value, and restrict ourselves to  $\nu = 0$ ,  $K_z = 0$  and  $(2m + 1) \ll b$ ,

so that  $\rho_m^2 = (2m + 1)/b \ll 1$ . We can estimate the size  $L_z$  of the atom along the  $z$ -axis and the energy  $\mathcal{E}_m$  for two different regimes of the values of  $R_K$ .

(i) For  $R_K \lesssim L_z \lesssim 1$  (but not necessarily  $R_K < \rho_m$ ) and with  $L_z$  as a variational parameter we have

$$\mathcal{E}_m \sim \frac{1}{L_z^2} - \frac{1}{L_z} \ln \frac{L_z^2}{\rho_m^2 + R_K^2} + \frac{mb}{M}, \quad (3.14)$$

where the first term is the kinetic energy along the  $z$ -axis, and the second term is the potential energy of the electron. The logarithmic factor in Eq. (3.14) comes from an integration over the “cigar-shaped” electron cloud in the displaced Coulomb potential  $-1/|\mathbf{r}' + \mathbf{R}_K|$ . Minimizing  $\mathcal{E}_m$  with respect to  $L_z$ , we obtain

$$L_z \sim \left( \ln \frac{1}{\rho_m^2 + R_K^2} \right)^{-1}, \quad \mathcal{E}_m \sim - \left( \ln \frac{1}{\rho_m^2 + R_K^2} \right)^2 + \frac{mb}{M}. \quad (3.15)$$

The mixing between different  $m$ -states is unimportant when  $b \gg b_{crit}$ . This can be seen from the order of magnitude estimate of the off-diagonal matrix element between  $m = 0$  and  $m = 1$  states:

$$\left\langle 0 \left| \frac{1}{|\mathbf{r}' + \mathbf{R}_K|} \right| 1 \right\rangle \sim \left\langle 0 \left| \frac{\mathbf{R}_K \cdot \mathbf{r}'}{r'^3} \right| 1 \right\rangle \sim \frac{R_K \hat{\rho}}{L_z (\hat{\rho}^2 + R_K^2)} \lesssim l, \quad (3.16)$$

as compared with  $\Delta \mathcal{E}_m \sim (l + b/M) \sim l(1 + b/b_{crit})$ . For  $b \lesssim b_{crit}$  the mixing is non-negligible, especially when  $R_K \sim \hat{\rho} \ll 1$ ; some results are given in Ref. [10]. When  $b \gg b_{crit}$ , the mixing can be neglected for all  $R_K$ .

(ii) For  $R_K \gtrsim 1$ , the Coulomb logarithm in Eq. (3.14) disappears, and we have (for  $m = 0$ ):

$$\mathcal{E}_0 \sim \frac{1}{L_z^2} - \frac{1}{(L_z^2 + R_K^2)^{1/2}}. \quad (3.17)$$

In the limit of  $R_K \gg 1$ , minimization of  $\mathcal{E}_0$  with respect to  $L_z$  yields

$$L_z \sim R_K^{3/4} \ll R_K, \quad \mathcal{E}_0 \sim -\frac{1}{R_K} = -\frac{b}{K_\perp}. \quad (3.18)$$

Thus for  $K_\perp \gtrsim b$ , the atom is very weakly bound ( $|\mathcal{E}_0| \lesssim 1$ ). The limiting scaling relations in Eq. (3.18) have been identified in [9,10].

We can calculate the energy eigenvalue more accurately. Substituting  $\phi(\mathbf{r}') = W_m(\mathbf{r}'_\perp)f_m(z)$  into  $H\phi(\mathbf{r}') = \mathcal{E}\phi(\mathbf{r}')$  with  $H$  given by Eq. (2.14), and averaging over the transverse direction, we obtain a one-dimensional Schrödinger equation

$$-\frac{1}{2\mu}\frac{d^2}{dz^2}f_m(z) + V_m(z, R_K)f_m(z) = \mathcal{E}_m f_m(z), \quad (3.19)$$

where the averaged potential is given by

$$V_m(z, R_K) = -\left\langle W_m(\mathbf{r}'_\perp) \left| \frac{1}{|\mathbf{r}' + \mathbf{R}_K|} \right| W_m(\mathbf{r}'_\perp) \right\rangle. \quad (3.20)$$

The function  $V_m(z, R_K)$  can be evaluated using an integral representation (e.g., [11])

$$V_m(z, R_K) = -\frac{1}{\hat{\rho}} \int_0^\infty dq \exp\left(-\frac{q^2}{2} - q\frac{|z|}{\hat{\rho}}\right) J_0(qR_K/\hat{\rho}) L_m\left(\frac{q^2}{2}\right), \quad (3.21)$$

where  $J_0$  is the Bessel function of zeroth order and  $L_m$  is the Laguerre polynomial of order  $m$  [34]. We solve for  $E$  by integrating Eq. (3.19) numerically from  $z = \infty$  to  $z = 0$  subject to the boundary conditions  $df/dz = 0$  at  $z = 0$  and  $f \rightarrow 0$  as  $z \rightarrow \infty$ . The energy eigenvalue  $\mathcal{E}_m$  as a function of  $R_K$  are shown in Figure 1 for  $B_{12} = 10$  and 100. Similar numerical results have also been obtained in Ref. [10]. For  $R_K \lesssim 1$ , we can fit the energy to a form similar to Eq. (3.15). The total energy of the  $m = 0$  state is then given by

$$\mathcal{E}_0(K_z, K_\perp) \simeq \frac{K_z^2}{2M} - 0.16 \left( \ln \frac{1}{\hat{\rho}^2 + CR_K^2} \right)^2, \quad (3.22)$$

and the atomic size  $L_z \sim 1/|\ln(\hat{\rho}^2 + CR_K^2)|$ . Equation (3.22) reduces to Eq. (3.2) for  $K_\perp = 0$ . From the numerical results we find  $C \simeq 0.8$ . For  $R_K \gtrsim 1$ , the binding energy of the atom is much smaller, and Eq. (3.22) should be replaced by the order of magnitude relation (3.18), while the actual numerical values of the energies are not important in practice (see Sec. V).

In the  $B \gg B_{crit}$  regime, the maximum value  $K_{\perp p}$  for the perturbation treatment of Sec. III.B to be valid becomes  $K_{\perp p} \sim b^{1/2}$  (cf. Eq. [3.8]). Thus for  $K_\perp \ll b^{1/2}$ , Eq. (3.22) should be consistent with Eq. (3.9). Indeed, when  $R_K \ll \hat{\rho}$ , Eq. (3.22) reduces to

$$\mathcal{E}_0(K_z, K_\perp) \simeq \frac{K_z^2}{2M} - 0.16 l^2 + 0.32 C \frac{l}{b} K_\perp^2. \quad (3.23)$$

The dependence on  $K_\perp$  is again quadratic, and the corresponding effective transverse mass is  $M_\perp \simeq b/(2ACl) \simeq 2b/l \simeq \xi b/l$ , in agreement with Eq. (3.10).

The  $m > 0$  states can be similarly calculated using Eqs. (3.19)-(3.21). Some numerical results are again shown in Figure 1. The energy can be expressed approximately as

$$\mathcal{E}_m(K_z, K_\perp) \simeq \frac{K_z^2}{2M} + m \frac{b}{M} - 0.16 \left( \ln \frac{1}{\rho_m^2 + C_m R_K^2} \right)^2. \quad (3.24)$$

From the numerical results we again obtain  $C_m \sim 1$ .

Comparison with the numerical results of Potekhin [10], who included the mixing of different  $m$ -states, indicates that Eqs. (3.22) and (3.24) are accurate to within  $\sim 30\%$  in the relevant regime of  $K_\perp$  ( $\lesssim b$ ) when  $b \gtrsim b_{crit}$ . The agreement becomes better as  $b$  increases. For smaller  $b$ , however, the perturbative results of Sec. 3.B should be adequate (see Sec. 3.D).

Finally, if we consider sufficiently strong magnetic field so that not only  $b/M \gtrsim l$  (or  $b \gtrsim b_{crit}$ ) but also  $b/M \gtrsim l^2$  is satisfied, then Eq. (3.24) implies that all the  $m > 0$  states are unbound, as has already been noted in Ref. [19]. However, this does *not* mean that there is no other bound state except a single non-degenerate  $m = 0$  state. Indeed, Eq. (3.22) indicates that there are many states for which the guiding centers of proton and electron are separated by a small  $R_K$ , and these states have similar energies compared to the ground state ( $m = 0, K_\perp = 0$ ). In the pseudomomentum scheme discussed here, these states occupy a continuum  $K_\perp$ -space. As we shall see in Sec. IV, these closely-packed energy levels can be made discrete if we use a different set of eigenstates.

#### D. General Fitting Formulae

Consider for the moment the cases with  $K_\perp \ll b$ , i.e.,  $R_K \ll 1$ , but with no other restrictions on  $K_\perp$  or  $b$ . In Sec. III.B-C, we have obtained reasonably accurate ground-state ( $m = 0$ ) energy of a hydrogen atom in two limiting regimes: (i) for  $B \ll B_{crit}$ , where Eqs. (3.9)-(3.10) are applicable up to adequately large values of  $K_\perp$ , and (ii) for  $B \gg B_{crit}$ , where the energy is given by Eq. (3.22). We write the total ground state energy in the form



$$\mathcal{E}_0(K_z, K_\perp) \simeq \frac{K_z^2}{2M} - 0.16 l^2 + E_\perp(K_\perp), \quad (3.25)$$

and want to find a general fitting formula for the “transverse kinetic energy”  $E_\perp(K_\perp)$  with  $K_\perp \ll b$ , but  $K_\perp/b^{1/2} = R_K/\hat{\rho}$  otherwise arbitrary. With the inequality  $R_K \ll 1$ , the second term in Eq. (3.22) can be approximated by  $-0.16 l^2 + 0.32 l \ln(1 + CR_K^2/\hat{\rho}^2)$ . We propose the following fitting formula

$$E_\perp(K_\perp) \simeq \frac{\tau}{2M_\perp} \ln \left( 1 + \frac{K_\perp^2}{\tau} \right), \quad \tau \simeq 0.64 \xi K_{\perp p}^2, \quad (3.26)$$

where  $M_\perp$  is given by Eq. (3.10). Recall that the parameter  $\xi \simeq 2 - 3$  for  $B_{12} = 0.1 - 10^3$ , and a typical number to use is  $\xi = 2.8$ . This formula reduces to Eq. (3.9) when  $K_\perp \ll K_{\perp p}$  and to the above approximation of Eq. (3.22) when  $B \gg B_{crit}$ . We expect Eq. (3.26) to be accurate to within 30% for  $K_\perp \ll b$ . In the regime  $b \gg b_{crit}$  and  $b \ll K_\perp^2 \ll b^2$  (i.e.,  $\hat{\rho} \ll R_K \ll 1$ ), Eq. (3.26) reduces to  $E_\perp \simeq 3.1 \ln(K_\perp^2/b)$  (a.u.)  $\gg 3$  (a.u.), which is large compared with the thermal energy (temperature)  $T$  for the astrophysical applications of interest. For evaluating the integral over  $K_\perp$  extending from zero to infinity in the atomic partition function (Sec. V), we shall advocate using Eq. (3.26) for all  $K_\perp$  even though this expression tends to infinity,<sup>2</sup> whereas the correct expression should approach the finite limit  $0.16 l^2$  for  $K_\perp \gg b$ . The difference is appreciable only where  $E_\perp \gg T$  (so that the Boltzman factor  $e^{-E_\perp/T}$  is very small) and our prescription amounts to “cutting off” the integral, i.e., omitting the states with  $R_K \gg 1$  from the integral. This omission is advantageous, since these states should be treated together with the ionized states, and both turn out to be unimportant (Sec. V).

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<sup>2</sup>A slightly more general fitting formula which closely resembles Eq. (3.22) is given by

$$\mathcal{E}_0(K_z, K_\perp) \simeq \frac{K_z^2}{2M} - 0.16 \left[ \ln \frac{b}{(1 + K_\perp^2/\tau)^\Gamma} \right]^2,$$

with  $\Gamma = 1 + Ml/(\xi b) = \tau/(0.64lM_\perp)$ . This expression can be applied to  $K_\perp \lesssim b$  and gives the correct limiting result for  $K_\perp \gg b$ , but it is not convenient to use in practice. For the applications discussed in Sec. V, Eqs. (3.25)-(3.26) are adequate.

Our fitting formulae for the energies of the  $m > 0$  states are less accurate. In the small- $K_\perp$  limit, the  $K_\perp$ -dependent term in Eq. (3.24) reduces to the quadratic form  $K_\perp^2/(2M_{\perp m})$ , with the effective mass given by Eq. (3.12). Similar to Eqs. (3.25)-(3.26) we fit  $\mathcal{E}_m$  to the analytical form:

$$\mathcal{E}_m(K_z, K_\perp) \simeq \frac{K_z^2}{2M} + m \frac{b}{M} - 0.16 l_m^2 + E_{\perp m}(K_\perp), \quad (3.27)$$

where

$$E_{\perp m}(K_\perp) \simeq \frac{\tau_m}{2M_{\perp m}} \ln \left( 1 + \frac{K_\perp^2}{\tau_m} \right), \quad \tau_m \simeq 0.64 \xi_m (2m+1)b \left[ 1 + \frac{M l_m}{\xi_m (2m+1)b} \right]^2, \quad (3.28)$$

so that  $E_{\perp 0} = E_\perp$ ,  $\tau_0 = \tau$ . Although  $\xi_m$  can vary by a factor of a few for different values of  $B$  and  $m$ , equation (3.28) has the correct approximate functional dependence for a wide range of  $B$  and  $K_\perp$ .

As noted in the introduction, one cannot construct a wave packet to mimic the classical behavior of a moving atom when both electron and proton are confined to the ground Landau level. Therefore when  $B \gg B_{crit} \gg B_o$ , the notion of “motion across the magnetic field” does not have a unique meaning. Nevertheless, one can ask two questions about the transverse pseudomomentum: (i) Is there an upper limit to  $K_\perp$  beyond which there is no bound state? (ii) When a bound state exists, what is the value of  $\mathbf{V}_\perp \equiv \partial \mathcal{E} / \partial \mathbf{K}_\perp$ , the analog to the classical center-of-mass transverse velocity of the atom? From our discussion in this section, we have seen that there exist bound states for all values of  $B$  and  $K_\perp$ , although the states with large  $K_\perp$  are very weakly bound. From Eq. (3.26), we have

$$\mathbf{V}_\perp \simeq \frac{\mathbf{K}_\perp}{M_\perp} \left( 1 + \frac{K_\perp^2}{\tau} \right)^{-1}. \quad (3.29)$$

(Note that for  $K_\perp \gg b$ , Eq. [3.18] should be used and we have  $V_\perp \sim b/K_\perp^2$  instead). Clearly, in general  $V_\perp$  is smaller than its field-free counterpart:  $V_\perp \simeq K_\perp/M_\perp$  (so that the effective mass description is valid) only for  $K_\perp < K_{\perp p}$ , and  $M_\perp \simeq M$  (classical behavior) only for  $b \ll b_{crit}$ . As  $K_\perp \rightarrow \infty$ , the center-of-mass velocity approaches zero. For a given magnetic field strength, the maximum  $V_\perp$  is given by

$$V_{\perp max} \simeq \frac{\tau^{1/2}}{2M_\perp} \sim \frac{K_{\perp p}}{M_\perp} \sim l b^{-1/2}, \quad (3.30)$$

which occurs when  $K_{\perp} \simeq \tau^{1/2} \sim K_{\perp p}$ . For  $b \gtrsim b_{crit}$ , the states with  $K_{\perp} \gg K_{\perp p}$  have not only small velocity but also large electron-proton separation  $R_K \gg \hat{\rho}$ . Nevertheless, these states are quite distinct from an electron-proton pair with separation  $R_K$  in fully ionized hydrogen, because the relative  $z$ -coordinate satisfies a bound-state wavefunction (localized, although with large scale-length and small binding energy). The partition function for these states is smaller than that for the ionized component, because the sum over the relative momentum in the  $z$ -direction,  $k_z$ , is absent.

#### IV. ALTERNATIVE APPROACH TO THE TWO-BODY PROBLEM

The basic states used in Sec. III for the e-p two-body problem are explicit eigenstates of the transverse pseudomomentum  $\mathbf{K}_{\perp}$ . For  $K_{\perp} = 0$ , this formulation has the advantages that the electron's "orbital" number  $m$  is a good quantum number, the wavefunction can be related to that for a fixed positive charge and the energy is given explicitly by Eq. (3.1). The  $K_{\perp} = 0$  states with different values of  $m$  are orthogonal to each other and could be used to satisfy the Pauli principle for the electrons in a hydrogen molecule [8,11] or a multi-electron atom [30]. The last term  $mb/M = m(b/b_{crit}) \ln b_{crit}$  in Eq. (3.1) is unimportant when  $b \ll b_{crit}$ , but it is very large when  $b \gg b_{crit}$  (and  $m \geq 1$ ). The simplest wavefunction for the  $H_2$ -ground state in this formulation would use one  $m = 0$  and one  $m = 1$  electron [8], and the energy would include the positive term  $(b/b_{crit}) \ln b_{crit}$ . One therefore might conclude that  $H_2$  has a positive energy relative to two H atoms when  $b \gg b_{crit}$ . In a future paper [11] we will show that this is not the case. In a molecule, only the total pseudomomentum is conserved, not that for individual atoms. Thus for  $b \gg b_{crit}$  one would have to perform an integral over  $K_{\perp}$  of individual atoms to form a molecular eigenstate (Similar situation exists for multi-electron atoms). To our knowledge this complicated task has not yet been carried out. We propose here an alternative set of basic states which are not eigenstates of the pseudomomentum. This formulation is more complex for single H atom, but can be generalized more easily to molecule. Moreover, this formulation makes the definition of

eigenstates clearer (unlike the pseudomomentum approach, where  $m$  is a good quantum only for  $K_\perp = 0$ ), and therefore offers an intuitive understanding of the degeneracy of states.

Let  $\mathbf{r}_1, \mathbf{r}_2$  be the position vectors of electron and proton in a H atom. We introduce coordinates  $Z = (m_e z_1 + m_p z_2)/M$  and  $z = z_1 - z_2$ , but stick to  $\mathbf{r}_{1\perp}$  and  $\mathbf{r}_{2\perp}$ . In this mixed coordinate system, the Hamiltonian for the electron-proton pair becomes  $H = H_o + V$ , with (cf. footnote 1):

$$H_o = \frac{K_z^2}{2M} + \frac{p_z^2}{2\mu} + \sum_{i=e,p} \frac{1}{2m_i} (\mathbf{p}_{i\perp} - e_i \mathbf{A}_i)^2, \quad (4.1)$$

where  $\mathbf{A}_i = \mathbf{A}(\mathbf{r}_i) = \mathbf{B} \times \mathbf{r}_{i\perp}/2$ , and the interaction potential is

$$V = -\frac{1}{[z^2 + (\mathbf{r}_{1\perp} - \mathbf{r}_{2\perp})^2]^{1/2}}. \quad (4.2)$$

We set  $K_z = 0$  without loss of generality.

Consider the transverse part of the wavefunction for a bound state. The Landau wavefunctions of the electron and proton form a complete set

$$W_{n_1 m_1}(\mathbf{r}_{1\perp}) W_{n_2 m_2}^*(\mathbf{r}_{2\perp}), \quad n_1, n_2, m_1, m_2 = 0, 1, 2, \dots \quad (4.3)$$

( $n_1, n_2$  specify the Landau excitations,  $m_1, m_2$  are the “orbital” quantum numbers as in Eqs. [2.3]-[2.4]). In general, an eigenstate of  $H$  can be constructed as

$$\Psi(z, \mathbf{r}_{1\perp}, \mathbf{r}_{2\perp}) = \sum_{n_1, m_1, n_2, m_2} W_{n_1 m_1}(\mathbf{r}_{1\perp}) W_{n_2 m_2}^*(\mathbf{r}_{2\perp}) f_{n_1 m_1 n_2 m_2}(z), \quad (4.4)$$

where we have restricted ourselves to  $z$ -wavefunctions without a node ( $\nu = 0$ ). Substituting Eq. (4.4) into the Schrödinger equation  $(H_o + V)\Psi = \mathcal{E}\Psi$  and using the orthogonal relations for the functions  $W$  to average over the transverse direction, we obtain a set of coupled differential equations from which the functions  $f(z)$ ’s and the eigenvalue  $\mathcal{E}$  can be calculated, at least in principle.

This set of equations is greatly simplified as a result of the conservation of total  $z$ -angular momentum  $J_z$ . Form Eq. (2.6), we have

$$J_z = -(m_1 - n_1) + (m_2 - n_2). \quad (4.5)$$

Indeed, since the basis function  $W_{n_1 m_1}(\mathbf{r}_{1\perp})W_{n_2 m_2}^*(\mathbf{r}_{2\perp}) \propto e^{-i(m_1 - n_1)\theta_1 + i(m_2 - n_2)\theta_2}$ , while the interaction potential  $V$  depend only on  $(\theta_1 - \theta_2)$ , we readily see that only the states with the same  $J_z$  are coupled.

We shall use the formalism of this section only when  $B \gg B_{crit}$ , in which case the Landau energy of the proton is large compared to the atomic Coulomb energy, so that both  $n_1$  and  $n_2$  become good quantum numbers. For astrophysical applications we are then interested in the ground Landau levels,  $n_1 = n_2 = 0$ . The energy eigenstate with a fixed  $z$ -angular momentum  $J_z = m_t = m_2 - m_1$  can be constructed as

$$\Psi^{(m_t)}(z, \mathbf{r}_{1\perp}, \mathbf{r}_{2\perp}) = \sum_{m_1} W_{m_1}(\mathbf{r}_{1\perp}) W_{m_t + m_1}^*(\mathbf{r}_{2\perp}) f_{m_1}^{(m_t)}(z). \quad (4.6)$$

The equations for the functions  $f$ 's are then given by

$$-\frac{1}{2\mu} \frac{d^2}{dz^2} f_{m_1}^{(m_t)}(z) - \sum_{m'_1} G_{m_1 m'_1}^{(m_t)}(z) f_{m'_1}^{(m_t)}(z) = \mathcal{E}^{(m_t)} f_{m_1}^{(m_t)}(z), \quad m_1 = 0, 1, 2, \dots \quad (4.7)$$

where

$$G_{m_1 m'_1}^{(m_t)}(z) = \langle W_{m_1}(\mathbf{r}_{1\perp}) W_{m_t + m_1}^*(\mathbf{r}_{2\perp}) | \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} | W_{m'_1}(\mathbf{r}_{1\perp}) W_{m_t + m'_1}^*(\mathbf{r}_{2\perp}) \rangle. \quad (4.8)$$

The set of equations (4.7)-(4.8) essentially forms a differential-integral equation system (the sum over  $m_1$  can be considered as an integration). Some mathematical formulae for evaluating the function  $G_{m_1 m'_1}^{(m_t)}(z)$  in Eq. (4.8) are given in Appendix A.

Since the states with different  $m_t$  are orthogonal, we can use the variational principle for each value of  $m_t$  separately to find a rigorous upper bound to  $E^{(m_t)}$ . To this end, we choose as a simple trial wavefunction the first term in Eq. (4.6), i.e., we include only  $m_1 = 0$ ,  $m_2 = m_t$ . Equation (4.7) then reduces to a single differential equation which is straightforward to solve numerically. For  $m_t = 0 - 4$ , we find that the upper bound can be written in the form:

$$\mathcal{E}^{(m_t)} < -0.16 A \left( \ln \frac{b/2.3}{C' m_t + 1} \right)^2, \quad (4.9)$$

with  $C' \simeq 0.9 - 1.1$  (depending on the values of  $m_t$ ), and  $A$  is a coefficient close to unity (as in Eq. [3.2]). This expression is equivalent to Eq. (3.22), with  $m_t^{1/2} \hat{\rho}$  playing the role of  $R_K$ ,

but here  $m_t$  is an integer. The form in Eq. (4.9) is expected since  $m_t = m_2 - m_1$  measures the difference between the distances to the origin of the guiding center of the electron and that of the proton. Although the  $m_t \geq 1$  state is not an exact  $K_\perp$ -eigenstate, in a qualitative sense the separation between electron and proton increases with increasing  $m_t$ . Thus we expect

$$G^{(m_t)}(z) \sim \frac{1}{[z^2 + (C'm_t + 1)\hat{\rho}^2]^{1/2}}, \quad (4.10)$$

which then naturally leads to the form in Eq. (4.9). The decrease from  $b$  in Eq. (3.2) to  $b/2.3$  in Eq. (4.9) arises from the fact that both the electron and proton wavefunctions have finite spread around the same axis (unlike the usual pseudomomentum approach, where the relative coordinate is used).

The actual energy eigenvalue  $\mathcal{E}^{(m_t)}$  can be obtained by solving iteratively the series of equations in (4.7) using the standard shooting algorithm [35]. We have carried out the calculations for the  $m_t = 0$  and  $m_t = 1$  states. Our numerical results are given in Figure 2 for three different values of field strength  $B_{12} = 100, 1000$  and  $5000$ . Typically, more than 10 terms in the sum of Eq. (4.6) are needed in order to attain convergence of the energy to within  $\lesssim 1\%$ . We find that the ground-state energy eigenvalue  $\mathcal{E}^{(0)}$  agrees with the standard value (Eq. [3.2] with  $m = 0$ ) in the limit of  $B \gg B_{crit}$ . This is expected because the  $m_t = 0$  ground state is also a  $K_\perp = 0$  eigenstate (Note that  $\mathbf{K}_{\perp 1} = -\mathbf{K}_{\perp 2}$  implies  $m_1 = m_2$  and hence  $m_t = 0$ ). Also, we see that as  $B$  increases, the upper bound given by Eq. (4.9) becomes asymptotically closer to the actual energy  $\mathcal{E}^{(m_t)}$ . For general  $m_t$ , we cannot give a rigorous lower bound to  $E^{(m_t)}$ , but it is approximately given by Eq. (4.9) with  $(b/2.3)$  replaced by  $b$ , so that the fractional uncertainty decreases as  $B$  increases. Note that although the contribution of the  $m_1 \geq 1$  terms in Eq. (4.6) to the correct energy becomes smaller as  $B$  increases, the contribution to the correct wavefunction is always non-negligible.

It is instructive to consider the degeneracy of an energy eigenstate. Without the Coulomb interaction between electron and proton, there is a double Landau degeneracy in  $m_1$  and  $m_2$ . When the Coulomb interaction is included, the degeneracy in  $m_t = m_2 - m_1$  is removed, but

a single degeneracy remains in  $m_1$ , i.e., for a given  $m_t$ , the eigenfunction corresponding to  $\mathcal{E}^{(m_t)}$  is not unique: the eigenstate in Eq. (4.6) with real  $f_{m_1}$ 's is presumably the state where the proton is centered at the origin; but there must be other states with the same energy, centered at different positions. We can demonstrate this degeneracy explicitly as follows. A Landau wavefunction centered at the origin of the coordinate can be expanded in terms of wavefunctions centered at some point  $\mathbf{r}_o = \mathbf{r}_{o\perp}$  as

$$W_{nm}(\mathbf{r}_\perp) = \sum_{m'} e^{i(m'-m)\theta_o} I_{n+m,n+m'} \left( \frac{r_o^2}{2\hat{\rho}^2} \right) e^{i\mathbf{K}_o \cdot \mathbf{r}_\perp / 2} W_{nm'}(\mathbf{r}_\perp - \mathbf{r}_o), \quad (4.11)$$

where  $\mathbf{r}_o \equiv x_o + iy_o = r_o e^{i\theta_o}$ ,  $\mathbf{K}_o$  is given by  $\mathbf{r}_o = -\mathbf{K}_o \times \mathbf{B} / B^2$  (see Eq. [2.2]),  $I_{n-m,n-m'}$  is the polynomial as defined in [37], and  $e^{i\mathbf{K}_o \cdot \mathbf{r}_\perp / 2}$  is the gauge factor. We consider only the ground Landau level  $n = 0$ , and write

$$W_m(\mathbf{r}_\perp) = e^{i\mathbf{K}_o \cdot \mathbf{r}_\perp / 2} \sum_{m'} C_m^{m'} W_{m'}(\mathbf{r}_\perp - \mathbf{r}_o), \quad (4.12)$$

where  $C_m^{m'}$  is a (complex) function of  $m$ ,  $m'$  and  $\mathbf{r}_o$ . The energy eigenstate in Eq. (4.6) can then be written as

$$\Psi^{(m_t)}(\mathbf{r}_1, \mathbf{r}_2) = e^{i\mathbf{K}_o \cdot (\mathbf{r}_{1\perp} - \mathbf{r}_{2\perp}) / 2} \sum_{m'_t} \left[ \sum_{m'_1} W_{m'_1}(\mathbf{r}_{1\perp} - \mathbf{r}_o) W_{m'_1+m'_t}^*(\mathbf{r}_{2\perp} - \mathbf{r}_o) f_{m'_1}^{(m_t m'_t)}(z) \right], \quad (4.13)$$

where we have defined

$$f_{m'_1}^{(m_t m'_t)}(z) \equiv \sum_{m_1} C_{m_1}^{m'_1} C_{m_1+m'_t}^{m'_1+m'_t} f_{m_1}^{(m_t)}(z). \quad (4.14)$$

However, the term inside  $[\dots]$  in Eq. (4.13) is exactly an energy eigenstate  $\Psi^{(m'_t)}(\mathbf{r}_1 - \mathbf{r}_o, \mathbf{r}_2 - \mathbf{r}_o)$  with  $J'_z = m'_t$  based on the coordinate system centered at  $\mathbf{r}_o$ . Since the state represented by the left-hand-side of Eq. (4.13) has a definite energy  $\mathcal{E}^{(m_t)}$ , while states with different  $m'_t$  have different energies, we must have  $m'_t = m_t$  in Eq. (4.13). Thus

$$\Psi_i^{(m_t)}(\mathbf{r}_1, \mathbf{r}_2) = e^{i\mathbf{K}_o \cdot (\mathbf{r}_{1\perp} - \mathbf{r}_{2\perp}) / 2} \Psi_j^{(m_t)}(\mathbf{r}_1 - \mathbf{r}_o, \mathbf{r}_2 - \mathbf{r}_o), \quad (4.15)$$

where we have added the subscripts “i, j” to indicate that there are many states associated with a given  $m_t$ , i.e., the states with the same energy  $\mathcal{E}^{(m_t)}$  is not unique. Clearly, the

degeneracy (per unit area) for a given  $m_t$  is  $B/(2\pi)$ , i.e., a single Landau degeneracy (see the discussion following Eq. [2.5]).

The above discussions demonstrate that there is a discrete set of states with  $m_t = 1, 2, 3, \dots$ , all having similar energies as the ground state ( $m_t = 0$ ), and do not have any positive contribution  $m_t b/M$  in their energies. This has important consequences for the binding of hydrogen molecules in the  $B \gg B_{crit}$  regime. In a forthcoming paper [11] we shall use one  $m_t = 0$  and  $m_t = 1$  atom to construct the wavefunction for the  $H_2$  ground state, which also does not involve any Landau excitation of the proton.

## V. IONIZATION-RECOMBINATION EQUILIBRIUM

### A. Overview

We now consider the ionization-recombination equilibrium of hydrogen atoms,  $e+p \rightleftharpoons H$ , given by the generalized Saha equation in the presence of a strong magnetic field. Previous treatments of this problem (e.g., [12–15]) either ignored the coupling between the center-of-mass motion and the internal atomic structure, or did not have available our generalized formula for the “transverse kinetic energy” as a function of the pseudomomentum  $K_\perp$ .

Let  $T$  be the gas temperature in atomic units (about  $3.16 \times 10^5$  K), so that the Boltzmann constant  $k_B$  is set equal to unity, and  $n_g$  be the number density (also in a.u.) of protons (either free or bound) in the gas. We write  $V_g = \pi R_g^3 \equiv 1/n_g$  and  $\mathcal{A}_g = \pi R_g^2$ , so that a “Wigner-Seitz cylinder” of radius and length  $R_g$  contains one proton on the average. Some of the partition function integrals can be simplified if the density and temperature satisfy three inequalities: (i) The density is low in the sense that  $R_g = (\pi n_g)^{-1/3}$  is much larger than the largest dimension (i.e., the  $z$ -dimension)  $L_z \sim l^{-1}$  of the ground-state atom; (ii) The temperature is much smaller than the ground-state binding energy  $|E_0| = |E(H)| \simeq 0.16 l^2 \gg 1$ ; (iii) The Coulomb attraction between a proton and an electron at typical separation  $R_g$  is of order  $R_g^{-1}$ ; we assume  $T \gg R_g^{-1}$  so that the “imperfect gas corrections”



are small.

The Saha equation involves the bound-atom partition function  $Z(H)$  compared with the product  $Z(e)Z(p)$  of the two free-particle partition functions. Each of these systems has six discrete or “nominally continuous” quantum numbers. Two of these for the free e-p system refer to the  $z$ -motion, which can be represented by  $K_z$ , the center-of-mass  $z$ -momentum and  $k_z$ , the relative  $z$ -momentum. For the bound system (H atom), the  $K_z$ -partition function is identical, but instead of  $k_z$  we have the quantum number  $\nu$ . In both systems the electron Landau excitations have the same quantum number  $n$  and energy  $nb$ , so that the  $n$ -partition functions are the same (In practice,  $b \gg T$ , so we only need to consider the ground Landau state of electron and the  $n$ -partition function is essentially unity). For the bound system, the remaining three quantum numbers are  $m$  and the two Cartesian components of the transverse pseudomomentum  $\mathbf{K}_\perp$ . For the free e-p system the three quantum numbers are  $n_2$ , the proton Landau level integer, and the two transverse parameters  $|K_{\perp 1}|$  and  $|K_{\perp 2}|$ .

## B. The Bound-State Partition Function of the H Atom

We first consider only the ground state of the H atom, with  $m = \nu = 0$ . Using Eq. (3.25), the canonical partition function in the volume  $V_g = R_g \mathcal{A}_g$  of a “Wigner-Seitz cylinder” can be written as

$$Z(H) \simeq R_g \left( \frac{MT}{2\pi} \right)^{1/2} \exp \left( \frac{|E(H)|}{T} \right) Z_\perp, \quad (5.1)$$

where the factor  $R_g(MT/2\pi)^{1/2}$  results from the free center-of-mass  $z$ -motion and  $|E(H)| = |E_0| \simeq 0.16 l^2$  is the ground-state binding energy. The partition function  $Z_\perp$  associated with the “transverse motion” of the atom has the form

$$Z_\perp = \frac{\mathcal{A}_g}{(2\pi)^2} \int_0^{K_{\perp max}} 2\pi K_\perp dK_\perp \exp \left[ -\frac{E_\perp(K_\perp)}{T} \right], \quad (5.2)$$

where  $E_\perp(K_\perp)$  is the generalized “transverse kinetic energy”. The upper limit  $K_{\perp max}$  of the integral in Eq. (5.2) is determined by the condition  $R_K \lesssim R_g$  so that the pressure-ionized

states are excluded in the bound state partition function. It thus has the density-dependent form  $K_{\perp max} \sim bR_g$ . As discussed in Sec. III.D,  $E_{\perp}$  is well approximated by Eq. (3.26) for  $K_{\perp}$  up to  $\sim b$ . However, for  $K_{\perp} \gg b$  (or  $R_K \gg 1$ ) the correct expression for  $E_{\perp}$  is close to  $0.16l^2$  (almost independent of  $K_{\perp}$ ), whereas the approximate  $E_{\perp}$  in Eq. (3.26) increases with  $K_{\perp}$ . At very low density ( $R_K \gg 1$ ), there are highly excited states with  $K_{\perp}$  between  $b$  and  $K_{\perp max} \sim bR_g$ , whose contribution to  $Z_{\perp}$  is proportional to  $\mathcal{A}_g b^2 n_g^{-2/3} \exp(-0.16l^2/T)$ . However, these states cover only a narrow range of binding energies (of order  $R_g^{-1} \ll T$ ) and can be neglected compared with the ionized components, in view of the inequality  $0.16l^2 \gg T$ . We can therefore omit these states entirely, but also make only a small error if we merely replace  $E_{\perp}$  by the approximation in Eq. (3.26), which is an overestimate for  $b \lesssim K_{\perp} \lesssim bR_g$ . This approximation has the advantage that the extension of the integral in Eq. (5.2) to infinity is not only finite but also small. We therefore get a convenient expression for  $Z_{\perp}$  by extending the integration to  $K_{\perp max} \rightarrow \infty$ . We have

$$Z_{\perp} \simeq \frac{\mathcal{A}_g}{2\pi} \int_0^{\infty} K_{\perp} dK_{\perp} \exp \left[ -\frac{\tau}{2M_{\perp}T} \ln \left( 1 + \frac{K_{\perp}^2}{\tau} \right) \right] = \mathcal{A}_g \frac{M'_{\perp}T}{2\pi}, \quad (5.3)$$

with

$$M'_{\perp} = M_{\perp} \left( 1 - \frac{2M_{\perp}T}{\tau} \right)^{-1}. \quad (5.4)$$

Thus  $Z_{\perp}$  is proportional to  $M'_{\perp}$ , which is larger than  $M_{\perp}$  (or equal to it when  $\tau/(2M_{\perp}T) \gg 1$ , so that the effective mass approximation is valid throughout the regime of interest), and  $M_{\perp}$  is larger than the actual mass  $M$ . While the transverse motion is “slowed down” in the sense that  $\partial E_{\perp}(K_{\perp})/\partial K_{\perp}$  is smaller than the zero-field result, the  $K_{\perp} \neq 0$  states still exist and their statistical weight  $\propto M'_{\perp}$  is actually increased over the zero-field result by the strong magnetic field.

We now consider the internal partition functions associated with the  $\nu > 0$  and  $m > 0$  excited states, i.e., we write the total bound-state partition function as

$$Z(H) = V_g \left( \frac{MT}{2\pi} \right)^{1/2} \frac{M'_{\perp}T}{2\pi} \exp \left( \frac{|E(H)|}{T} \right) z_{\nu}(H) z_m(H). \quad (5.5)$$

Start with the quantum number  $\nu$ . The internal partition function relative to the ground state is

$$z_\nu(H) \simeq 1 + \exp\left(-\frac{|E_0|}{T}\right) \sum_{\nu=1}^{\nu_{max}} 2 \exp\left(\frac{|E_\nu|}{T}\right). \quad (5.6)$$

Here  $E_\nu$  is given by Eqs. (3.4)-(3.5) but can be approximated by  $E_\nu = -1/(2\nu^2)$ , and the factor of 2 comes from the near-degeneracy of the even and odd states. The sum in Eq. (5.6) is thus similar to that for a field-free atom except that the usual weight-factor  $2\nu^2$  is missing as the atom is one-dimensional. Since  $|E_0| - |E_\nu| \gg T$  for the temperature regime of interest, the individual term in the sum is very small, but the  $z_\nu(H)$  would diverge if  $\nu_{max}$  were allowed to become infinite. As for the high Rydberg states in the field-free H atom, the divergence is avoided by including only states which fit inside the Wigner-Seitz cylinder. The size of the  $\nu \geq 1$  state is  $L_z \sim \nu^2$  (a.u.), so we should choose  $\nu_{max} \sim R_g^{1/2}$  with energy  $E_{\nu_{max}} \simeq -1/(2R_g)$ , i.e., we omit states with such extended wavefunctions that they would be pressure-ionized. With this prescription the sum in Eq. (5.6) becomes finite but density-dependent, i.e., it increases as  $n_g^{-1/6}$  with decreasing  $n_g$ . Making use of the inequality  $T \gg R_g^{-1} \simeq 2|E_{\nu_{max}}|$ , we split the sum into two parts: one extends from  $\nu = 1$  to  $\nu_T$ , where  $|E_{\nu_T}| = T$ ; the other from  $\nu_T$  to  $\nu_{max}$  (which exceeds  $\nu_T$  because of the inequality). The first part contains only a few terms, each with  $|E_0| - |E_\nu| \gg T$ , so they can be neglected (compared with unity, coming from the  $\nu = 0$  term). The second part represents the highly excited states and would contribute approximately  $2 \exp(-|E_0|/T)(\pi n_g)^{-1/6}$ , which could be large for very small density  $n_g$ . However, these states should be considered separately and compared with the ionized components: These states have negative energies of order  $(-1/R_g)$ , while the ionized components have positive energies of order  $T$ . Because of the inequality  $T \gg R_g^{-1}$ , we neglect these states entirely in the rest of the paper and set  $z_\nu(H) \simeq 1$ .

The contribution of the  $m > 0$  states to the bound-state partition function can be considered in the same manner as that of the  $m = 0$  state discussed before. The internal

partition function associated with the  $m$ -states is given by <sup>3</sup>

$$z_m(H) \simeq \left(1 + e^{-b/MT}\right) \sum_{m=0}^{\infty} \frac{M'_{\perp m}}{M'_\perp} \exp \left[ -\frac{1}{T} \left( 0.16 l^2 - 0.16 l_m^2 + m \frac{b}{M} \right) \right], \quad (5.7)$$

where

$$M'_{\perp m} = M_{\perp m} \left( 1 - \frac{2M_{\perp m}T}{\tau_m} \right)^{-1}, \quad (5.8)$$

so that  $M_{\perp 0} = M_\perp$  (cf. Eq. [5.4]), and  $M_{\perp m}$ ,  $\tau_m$  are given in Eqs. (3.12) and (3.28). The sum in Eq. (5.7) simplifies in two extreme regimes of the field strength: For  $b \ll b_{crit}$  one may need to include a number of terms in the sum, but then  $M'_{\perp m}$  is close to  $M$ ; For  $b \gg b_{crit}$  the effective mass  $M'_\perp$  is much larger than  $M$ , but since  $b \gg MT$  one need to include only the  $m = 0$  ground state, and hence  $z_m(H) = 1$ .

Finally, it is instructive to consider the partition function based on the alternative scheme discussed in Sec. IV. Using Eq. (4.9) (and relacing  $b/2.3$  by  $b$ ; see the discussion following Eq. [4.10]), we see that  $Z(H)$  can still be written as Eq. (5.1), but the transverse partition function  $Z_\perp$  is now given by

$$Z_\perp \sim \frac{\mathcal{A}_g b}{2\pi} \sum_{m_t=0}^{m_{t,max}} \exp \left[ -\frac{l}{T} \ln(1 + C' m_t) \right] \sim \frac{\mathcal{A}_g b}{2\pi} \int_0^{m_{t,max}} dm_t (1 + C' m_t)^{-l/T}, \quad (5.9)$$

where the factor  $\mathcal{A}_g b/2\pi$  comes from the Landau degeneracy of the  $m_t$ -th state, and  $m_{t,max} \sim R_g^2 b$ . Clearly, Eq. (5.9) has the same form as Eq. (5.3) in the limit of  $b/M \gg l$ , demonstrating the equivalence of the two energy level schemes of Sec. II-III and Sec. IV.

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<sup>3</sup>The factor  $(1 + e^{-b/MT})$  in Eq. (5.7) results from the proton spin term, which is not explicitly included in our calculations (see footnote 1). Note that when the proton spin term (but not the abnormal magnetic moment) is taken into account in Eq. (2.11) or (2.13), the energy of the  $m$ -th atomic state is given by  $\mathcal{E}_m \simeq K_z^2/(2M) - 0.16 l_m^2 + E_{\perp m}(K_\perp) + mb/M + (1 + \sigma_z)b/(2M)$ , where the proton spin  $\sigma_z = \pm 1$  (compare with Eq. [3.27]).

### C. Saha Equation

The partition function of the free electrons in the ground Landau level is given by

$$Z(e) \simeq R_g \left( \frac{T}{2\pi} \right)^{1/2} \left( \mathcal{A}_g \frac{b}{2\pi} \right), \quad (5.10)$$

where the factor  $R_g(T/2\pi)^{1/2}$  represents the free  $z$ -motion and the factor  $\mathcal{A}_g b/(2\pi)$  is the Landau degeneracy. For the free protons (see footnote 1), we have

$$\begin{aligned} Z(p) &= R_g \left( \frac{MT}{2\pi} \right)^{1/2} \left( \mathcal{A}_g \frac{b}{2\pi} \right) \sum_{n_2=0}^{\infty} g_{n_2} \exp \left( -\frac{n_2 b}{MT} \right) \\ &= V_g \left( \frac{MT}{2\pi} \right)^{1/2} \frac{b}{2\pi} \left[ \tanh \left( \frac{b}{2MT} \right) \right]^{-1}, \end{aligned} \quad (5.11)$$

where the sum extends over all Landau levels of the proton, and  $g_{n_2}$  is the spin degeneracy:  $g_{n_2} = 1$  for  $n_2 = 0$  and  $g_{n_2} = 2$  for  $n_2 > 0$ . Given  $Z(e)$ ,  $Z(p)$  and  $Z(H)$ , the ionization-recombination equilibrium can be obtained using the condition  $\mu(e) + \mu(p) = \mu(H)$  for the chemical potentials. In the density and temperature regimes of interest, with  $T \ll K_{\perp p}^2/(2M_{\perp})$ , we have

$$\frac{X(H)}{X_p X_e} \simeq n_g \left( \frac{b}{2\pi} \right)^{-2} M_{\perp} \left( 1 - \frac{2M_{\perp} T}{\tau} \right)^{-1} \left( \frac{T}{2\pi} \right)^{1/2} \tanh \left( \frac{b}{2MT} \right) \exp \left( \frac{|E(H)|}{T} \right) z_m(H), \quad (5.12)$$

where  $X(H) = n(H)/n_g$ ,  $X_p = n_p/n_g$ ,  $X_e = n_e/n_g$  are the number density fraction of different species,  $M_{\perp} = M + \xi b/l$  (with  $\xi \simeq 2.8$ ), and  $z_m(H)$  is given by Eq. (5.7). This is the generalized Saha equation in the presence of a superstrong magnetic field. More details on the applications of this result to neutron star atmospheres will be presented elsewhere [36].

### VI. SUMMARY

The effects of center-of-mass motion of neutral hydrogen atom in a strong magnetic field are rather intricate, mainly due to the high degree of degeneracy associated with the

quantum states. Using the usual pseudomomentum scheme (Sec. II-III), we have obtained approximate solutions for the energy of the atom as a function of the field strength and conserved pseudomomentum for a wide range of parameter regimes. In particular, we have considered field strengths  $B \gtrsim B_{crit} \sim 4 \times 10^{13}$  G, when the Landau excitation energy of proton is considerable. States with large transverse pseudomomentum have small binding energy and transverse velocity, but are nevertheless quite distinct from fully ionized states. We have concentrated on convenient analytic fitting formulae which give at least a reasonable approximation over various parameter regimes (see particularly Eq. (3.26) for the “transverse kinetic energy”). Since there may be neutron star atmospheres with  $B \sim 10^{13} - 10^{14}$  G, we are particularly interested in the cases with  $B \gg B_{crit}$ , where the proton Landau energy  $\hbar\omega_p$  is very large. By considering an alternative scheme to the usual pseudomomentum formulation (Sec. IV), we have shown that there are atomic states with orbital wavefunctions orthogonal to that of the ground state, but without any Landau excitation appearing in their energies.

We have also derived the generalized Saha equation for the equilibrium between neutral hydrogen atoms and the ionized component. We focused on the cases of astrophysical interest, where the density is relatively low and the thermal energy  $k_B T$  is small compared to the atom’s ground state binding energy. Although the maximum transverse velocity of bound atoms is small in strong magnetic fields, the statistical weight due to transverse motion is actually increased by the strong fields, not decreased (Sec. V). The statistical weight of highly excited bound states is smaller than that of the fully ionized component. Our results are important for determining the physical conditions of magnetic neutron star atmospheres as well as the soft X-ray (or EUV) radiation spectra from them. Some of these issues will be studied in a future paper [36].

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## APPENDIX A:

In this Appendix, we derive some mathematical formulae needed for evaluating the function  $G_{m_1 m'_1}^{(m_t)}(z)$  defined by Eq. (4.8). (Here the lengthscale is in units of the cyclotron radius  $\hat{\rho}$ .) Using the identity

$$\frac{1}{r} = \frac{1}{2\pi^2} \int \frac{d^3 q}{q^2} e^{i\mathbf{q} \cdot \mathbf{r}}, \quad (\text{A1})$$

we write Eq. (4.8) as

$$G_{m_1 m'_1}^{(m_t)}(z) = G_{m'_1 m_1}^{(m_t)}(z) = \frac{1}{2\pi^2} \int \frac{d^3 q}{q^2} e^{iq_z z} \langle m_t + m_1 | e^{i\mathbf{q}_\perp \cdot \mathbf{r}_{1\perp}} | m_t + m'_1 \rangle \langle m'_1 | e^{-i\mathbf{q}_\perp \cdot \mathbf{r}_{2\perp}} | m_1 \rangle. \quad (\text{A2})$$

Using the general result [37] for the matrix element  $\langle m' | e^{i\mathbf{q}_\perp \cdot \mathbf{r}_\perp} | m \rangle$ , and integrating over  $dq_z$ , we obtain (assuming  $m_1 \geq m'_1$  without loss of generality):

$$G_{m_1 m'_1}^{(m_t)}(z) = \int_0^\infty dq e^{-q|z|-q^2} \left(\frac{q^2}{2}\right)^{m_1-m'_1} \sqrt{\frac{(m_t+m'_1)! m'_1!}{(m_t+m_1)! m_1!}} L_{m_t+m'_1}^{m_1-m'_1}\left(\frac{q^2}{2}\right) L_{m'_1}^{m_1-m'_1}\left(\frac{q^2}{2}\right), \quad (\text{A3})$$

where  $L_n^m$  is the Laguerre polynomial of order  $n$  [34]. We now define constant coefficients  $g_n^{(m_t)}(m_1, m'_1)$  via

$$\left(\frac{x}{2}\right)^{m_1-m'_1} \sqrt{\frac{(m_t+m'_1)! m'_1!}{(m_t+m_1)! m_1!}} L_{m_t+m'_1}^{m_1-m'_1}\left(\frac{x}{2}\right) L_{m'_1}^{m_1-m'_1}\left(\frac{x}{2}\right) = \sum_{n=0}^{m_1+m'_1+m_t} g_n^{(m_t)}(m_1, m'_1) L_n(x). \quad (\text{A4})$$

Using the relation

$$V_n(z) = \int_0^\infty dq e^{-q^2/2-q|z|} L_n\left(\frac{q^2}{2}\right) = \frac{1}{\sqrt{2}n!} \int_0^\infty dx \frac{x^n e^{-x}}{(x+z^2/2)^{1/2}}, \quad (\text{A5})$$

where the second equality can be used to evaluate the function  $V_n(z)$ , we obtain

$$G_{m_1 m'_1}^{(m_t)}(z) = \sum_{n=0}^{m_1+m'_1+m_t} \frac{1}{\sqrt{2}} g_n^{(m_t)}(m_1, m'_1) V_n\left(\frac{z}{\sqrt{2}}\right). \quad (\text{A6})$$

We calculate the coefficients  $g_n^{(m_t)}(m_1, m'_1)$  using the orthogonal relations of Laguerre polynomials. We can identify two special cases: (i) When  $m_t = 0$ , we have  $G_{m_1 m'_1}^{(0)}(z) = E_{m_1 m'_1}(z)$  and  $g_n^{(0)}(m_1, m'_1) = e_n(m_1, m'_1)$ , where  $E_{m_1 m'_1}(z)$  and  $e_n(m_1, m'_1)$  are given in [8]; (ii) When  $m_1 = m'_1 = 0$ , we have  $G_{00}^{(m_t)}(z) = D_{0m_t}(z)$  and  $g_n^{(m_t)}(0, 0) = d_n(0, m_t)$ , where  $D_{m_1 m'_1}(z)$  and  $d_n(m_1, m'_1)$  are again given in [8].

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## FIGURES

FIG. 1. Numerical results for the energies of hydrogen atom in the  $m = 0$  state (solid lines) and  $m = 1$  state (dotted lines) as a function of  $R_K$ , obtained by solving Eq. (3.19). The upper curves are for  $B_{12} = 10$ , and the lower curves for  $B_{12} = 100$ .

FIG. 2. The energy eigenvalue  $\mathcal{E}^{(m_t)}$  calculated from Eq. (4.7) for the  $m_t = 0$  (upper panel) and  $m_t = 1$  (lower panel) states. The ratio  $\mathcal{E}^{(m_t)}/E_o$ , where  $E_o = -0.16 A l^2$  is the ground-state energy as given by Eq. (3.2), is plotted against  $m_{1max}$ , the maximum values of  $m_1$  in the sum of Eq. (4.6). The filled triangles are for  $B_{12} = 100$ , the open circles for  $B_{12} = 1000$ , and the filled circles for  $B_{12} = 5000$ .



